



The DOE Center of Excellence for The Synthesis and Processing of Advanced Materials



Basic Energy Sciences
Division of Materials Sciences and Engineering

http://www.sandia.gov/1100/XCSP/xcsp_homepage.htm

*A model of integration within the DOE as well as of collaborations
among the participating institutions*

Center Review

Germantown, MD, June 12, 2003

OVERVIEW

Outline

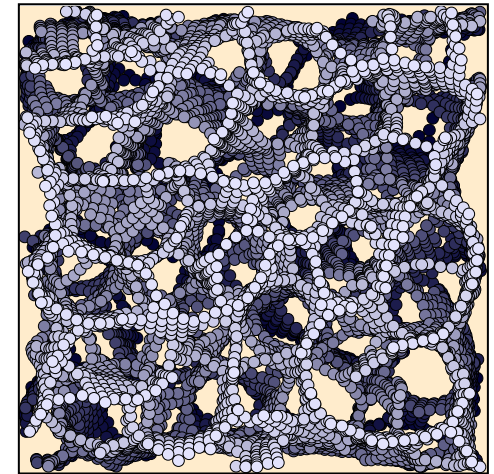
- Center and its Objective
- Current Center Projects
- Recent Project Changes
- Some Reflections

The DOE Center of Excellence for The Synthesis and Processing of Advanced Materials



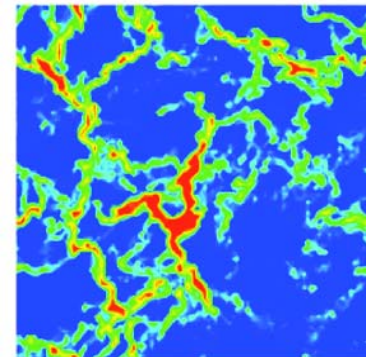
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Nano-Scale Magnets



Simulated nanocomposites formed in a
triaxial field

Granular Flow



Density inhomogeneities in freely
evolving granular gas

- A coordinated/cooperative venture among
 - 12 DOE Labs
 - University Grant Research
 - Industrial Collaborators
- *Objective*
To enhance the science and engineering of materials synthesis and processing in order to meet the programmatic needs of the Department of Energy and to facilitate the technological exploitation of materials.
- Capitalizes on the complementary strengths of the participating institutions to solve important problems and add value

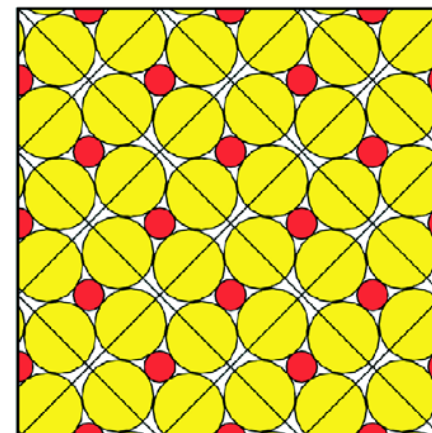
Multi-Lab Center Projects Emphasize Scientific Excellence & Technological Relevance



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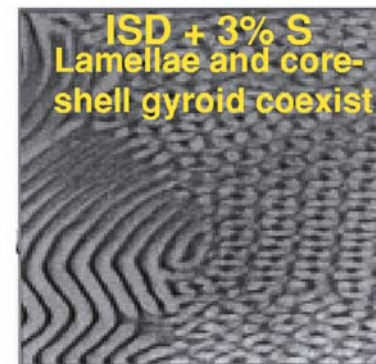
- Isolated and Collective Phenomena in Nanocomposite Magnets
- Controlled Defect Structures in Rare-Earth Ba-Cu-O Cuprate Superconductors
- The Science of Localized Corrosion
- Smart Structures Based on Electroactive Polymers
- Nanoscale Phenomena in Perovskite Thin Films
- Granular Flow and Kinetics
- Synthesis and Processing of Carbon-based Nanostructured Materials
- Experimental and Computational Lubrication at the Nanoscale

Perovskite Thin Films



TiO₂ layer on PbTiO₃ (001)

Electroactive Polymers



200 nm

Polymer Hybrid Morphology

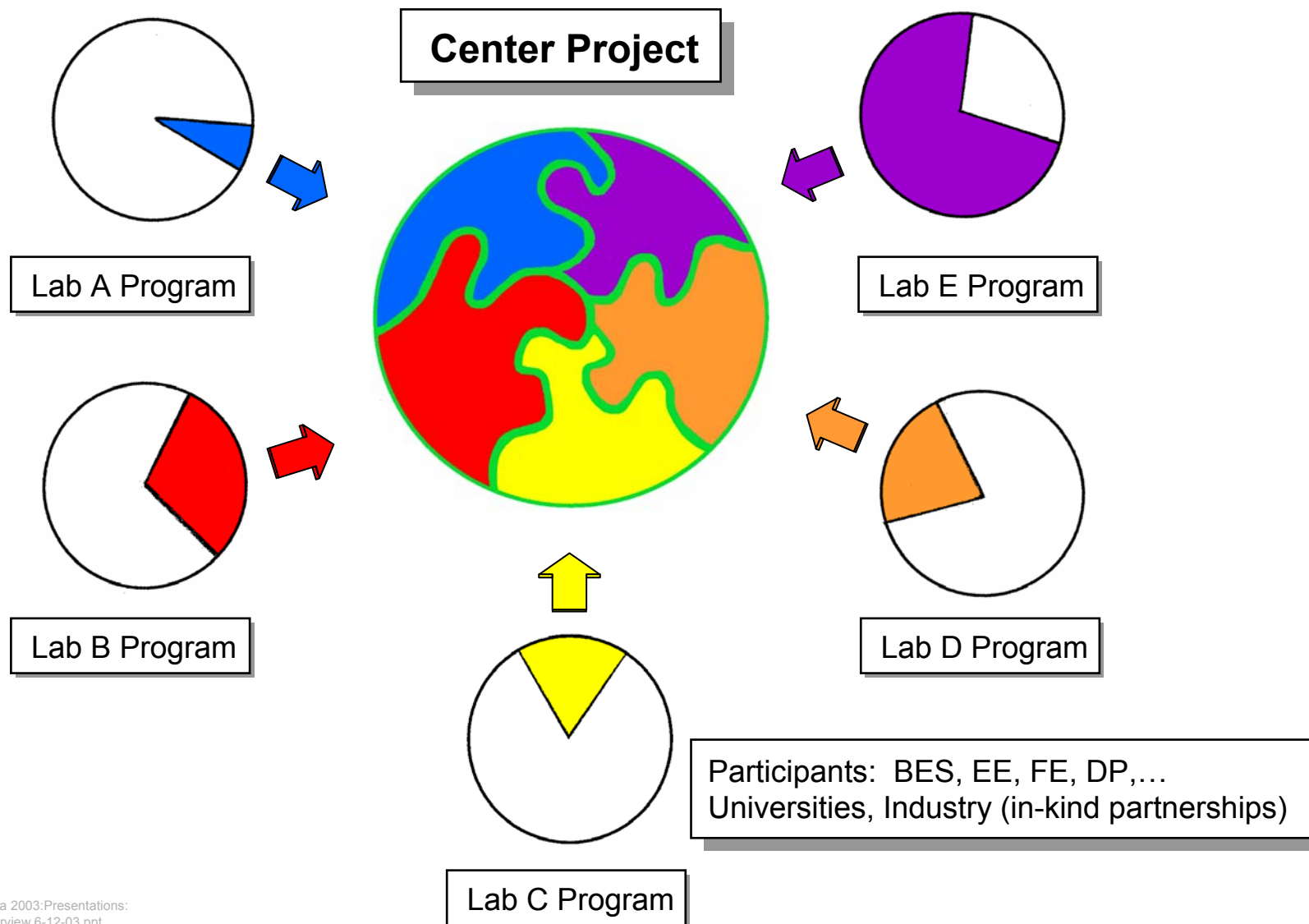
Selection Criteria

- **Scientific excellence**
- **Clear relationship to energy-related technologies**
- **Involvement of several laboratories**
- **Existing or potential partnerships with DOE Technologies-funded programs**
- **Existing or potential in-kind partnerships with industry**

Center Projects Build on Selected Activities from On-Going Research Programs at the Laboratories



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CSP PROJECTS

FY'03 “Glue” Funding Summary

Project Lab	Localized Corrosion	Nano Magnets	Cuprate Super-conductors	Perovskite Films	Electroactive Polymers	Granular Flow	Carbon Nanostructures	Nanoscale Lubrication
Ames	20 (03-01)	25 (01-01) 25 (02-02)	50 (01-05)		20 (03-02)	120* ^a (02-03)		
ANL		55 (02-02)	60 (01-05)	135* ^b (01-03)	30 (03-01)	70 (02-02)	110* ^c (03-01)	20 (03-01)
BNL	25 (01-03)	35 (02-02)	65 (02-03)		25 (03-02)			
INEEL		25 (02-02)			20 (01-05)			
UI/MRL	20 (01-01)	15 (01-03)			36 (02-02)			70 (01-03)
LBNL		25 (02-02)			16 (03-01)		27.5 (01-01)	25 (03-01)
LLNL	20 (01-02)	10 (03-01)			21 (02-03)			
LANL		20 (01-05)	40 (02-01)	25 (02-02)		70 (02-01)		20 (01-05)
NREL								
ORNL		20 (01-02)	60 (02-02)	80 (01-03)	30 (03-01)		67.5 (02-02)	55 (01-01)
PNNL	20 (01-02)				68* ^d (01-05)			30 (01-01)
SNL/CA								
SNL/NM	145* ^e (01-03)	20 (03-01)	25 (01-05)	25 (01-01)	34 (03-01)	40 (01-02)	67.5 (01-05)	55 (01-02)
TOTAL (\$K)	250* ^f	275* ^g	300	265* ^h	300	300	272.5* ⁱ	275* ^j

Includes \$75 K for university grants and workshops.

Include \$10 K for Univ. of Florida and \$10K for Univ. of Maryland.

Includes \$27.5 K subcontract to NCSU (Nemanich).

Includes \$25 K for university subcontracts.

Includes \$50 K to Ohio State University and \$50 K to University of Utah.

Remaining \$50 K should be sent directly to Prof. Rob Kelly, Univ. of Virginia via Prof. John Scully's existing BES contract.

Remaining \$25 K should be sent to Prof. Kannan Krishnan, University of Washington on his new BES contract.

Remaining \$35K should be sent directly to Prof. Dravid, Northwestern Univ. who is supported by DMS under KC 02-01-01.

Remaining 27.5 K should be sent directly to Prof. Dravid, Northwestern Univ. who is supported by DMS under KC 02-01-01.

Remaining \$25 K should be sent directly to Prof. S. Sinha at UC/SD.

Recent Project Changes



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Graduated at End of FY02

- Design and Synthesis of Ultrahigh Temperature Intermetallics

Started at Beginning of FY03

- Experimental and Computational Lubrication at the Nanoscale

Experimental and Computational Lubrication at the Nanoscale



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Objectives

- *Develop a scientific understanding of lubrication and strategies to control tribology at the nanoscale capitalizing on recent advances in nanoprobe, theoretical and computational methods.*

Tasks

- Confined Water/Non-polar Fluids/Patterned Surfaces and Lubrication
- Development of New Probe Methods
- New theory and Computation Related to Experiments

Participants. ANL, LANL, LBNL, ORNL, SNL/NM, UI/FS-MRL, UCSD

Coordinator. Steve Granick (UI/FS-MRL), (217) 333-5720, sgranick@uiuc.edu

Sponsoring/Collaborating Organizations

BES/DMS&E

DOE/OTT

DOE/DP

Interactions w/~12 Companies

Current Center Projects



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Start and Graduation Dates	<u>Start</u>	<u>Graduation</u>
▪ The Science of Localized Corrosion	FY 99	FY 03
▪ Isolated and Collective Phenomena in Nanocomposite Magnets	FY 00	FY 04
▪ Controlled Defect Structures in Rare-Earth Ba-Cu-O Cuprate Superconductors	FY 00	FY 04
▪ Smart Structures Based on Electroactive Polymers	FY 01	FY 05
▪ Nanoscale Phenomena in Perovskite Thin Films	FY 01	FY 05
▪ Granular Flow and Kinetics	FY 02	FY 06
▪ Synthesis and Processing of Carbon-Based Nanostructured Materials	FY 02	FY 06
▪ Experimental and Computational Lubrication at the Nanoscale	FY 03	FY 07

Graduated Project Design and Synthesis of Ultrahigh-Temperature Intermetallics



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Division of Materials Sciences and Engineering

Objectives

- *Generate the knowledge required to establish a scientific basis for the design and processing of transition-metal silicides and materials based on silicides for structural applications at temperatures of 1400°C and above.*

Tasks

- First Principles Calculations/Simulations
- Structure and Properties
- Processing and Fabrication

Focus: Mo_5Si_3 -base Alloys

Participants

- Ames, ANL, INEEL, LBNL, LLNL, LANL, ORNL, SNL/CA, UI/MRL

Coordinators

- R. Judkins, ORNL, (423) 574-4572/judkinsrr@ornl.gov, R. B. Thompson, Ames (515) 294-8152 thompsonrb@cnde.iastate.edu

Sponsoring/Collaborating Organizations

BES/DMS&E

FE/AR&TD

EE/AIM

Graduated Project

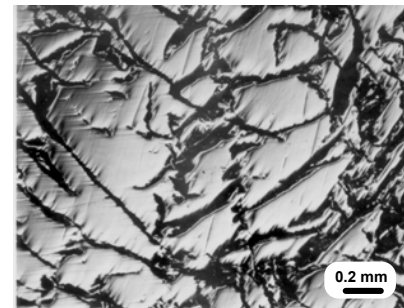
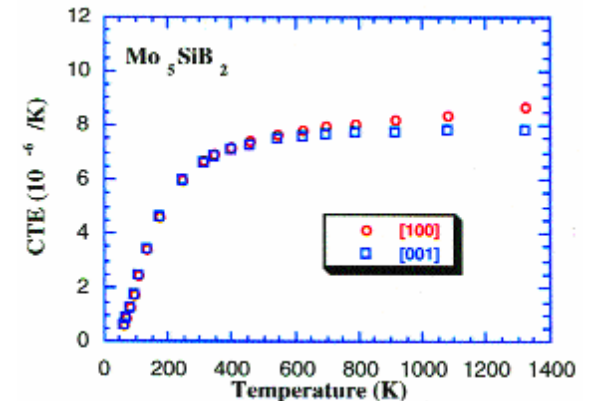
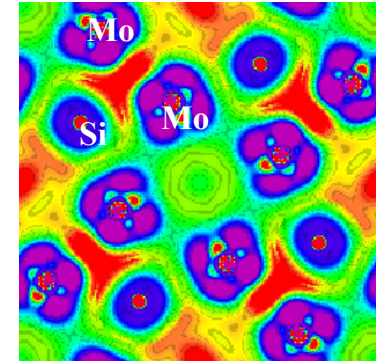
Design and Synthesis of Ultrahigh-Temperature Intermetallics



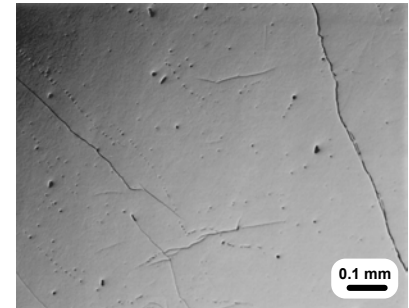
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Highlights

- First-principles calculations established the nature of the bonding in Mo_5Si_3 and revealed the influence of alloying (B, Al) on phase behavior, thermal expansion anisotropy and elastic properties.
- Alloying results agree with calculations
 - Al retains T1 phase; large CTE anisotropy; grain boundary cracking
 - B \rightarrow T₂ phase; 30% higher hardness and fracture toughness; reduced CTE anisotropy; greatly reduced cracking; improved processing
 - Nb and V reduce CTE



Mo_5Si_3



$(\text{Mo}_{0.4}\text{Nb}_{0.6})_5\text{Si}_3$

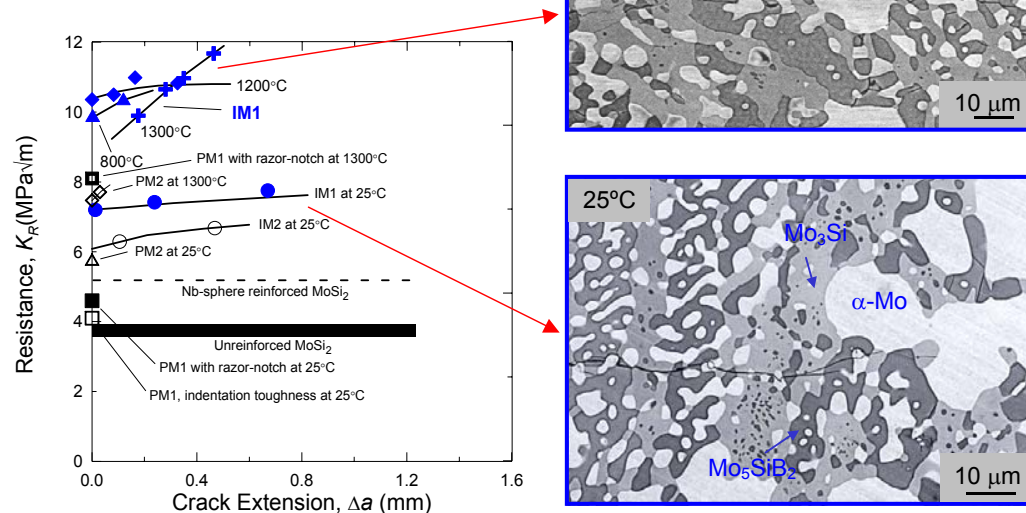
Graduated Project

Design and Synthesis of Ultrahigh-Temperature Intermetallics



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Highlights



- A process to improve the fracture toughness of Mo-Si-B alloys was developed and demonstrated. The process is based on the consolidation of Mo-coated Mo-Si-B particles leading to the formation of Mo_3Si and Mo_5SiB_2 phases in a continuous α -Mo matrix.

- Shown that the boron-modified molybdenum silicide alloy, Mo-12Si-8.5B (at.%), can be processed to be considerably tougher and more fatigue resistant than both monolithic MoSi_2 and Nb-sphere reinforced MoSi_2 . Additionally, the crack-growth resistance of this B-modified alloy increases progressively with increasing temperature up to 1300°C.

Graduated Project

Design and Synthesis of Ultrahigh-Temperature Intermetallics



Highlights

- Stress-strain properties and dislocation structure studies on T2 Mo-Si-B alloys produced by powder metallurgy exhibit high plasticity above 1400°C as well as high strength (140 MPa at 10^{-4} /s).
- The high temperature strength of Mo-Si-B alloys was shown to depend strongly on the topology and scale of the alloy's microstructure. For comparable compositions, the creep strength can be varied by as much as a factor of two by manipulating the microstructure and its scale.
- Showed that a protective scale forms on Mo-Si-B alloys during isothermal oxidation that significantly reduces oxygen transport and the formation of Mo and MoO₂ precipitates at the scale/alloy interface. These borosilicate scales as well as sulfide scales formed during sulfidation experiments may greatly improve oxidation and corrosion resistance.



2 Proposals were received in response to the call and were reviewed at the MRS Fall Meeting

- Spin Polarized Transport in Complex Oxides*
- Defect Studies in Wide Bandgap Semiconductors

* Selected for FY04 start



Objectives

- *Understand, control and manipulate spin-polarized transport within and between highly spin-polarized oxides in order to create and exploit spintronic functionality.*

Tasks

- Synthesis & Processing: Tailoring Interfacial Chemistry and Structure
- Spin Transport Across and Along Interfaces
- New Theory and Computation Related to Experiments

Participants

- ANL, BNL, LANL, LLNL, ORNL, UI/FS-MRL, Cornell, Univ. of Tennessee

Coordinator

- John Mitchell, ANL, (630) 252-5852, mitchell@anl.gov

Sponsoring/Collaborating Organizations

BES/DMS&E

DOE/DP

Motorola

IBM

Defect Studies in Wide Bandgap Semiconductors



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Objectives

- *Improve the light-emitting efficiency of wide bandgap semiconductors through a better understanding and control of defects, impurities and dopants.*
 - Aimed at Solid State Lighting
 - Emphasis on Ga N – based materials
 - Strong coupling between experiments and theory

Team held planning meeting at 2003 Spring MRS



- You need a sharp focus on one theme with common/similar materials. Fosters cooperation, collaborations, joint publications/presentations.
- Collaborations integrated unique capabilities and expertise.
- Collaborative efforts with universities, industry and others were very relevant and useful.
- Diversity of skills, approaches, and interests among participants presented challenges to coordination early on,
but
yielded opportunities to do/see things differently and added value.
- Face-to-face informal coordination meetings very valuable (~2/yr).
- The “glue” was very valuable in furthering/cementing collaborations.
- Labs’ researchers want to be involved in CSP.

- **Project Selection Criteria**

Clear Relation to Energy Related Technologies

“Improving connections to DOE Technologies is very desirable”

“Strengthen the vision that BES has an important role in basic materials science”

but

“Do not push the connection to energy too far”

“Keep the fundamental aspects of the work visible”

“Do not push BES programs into applications”

- **More visibility for CSP and its work**

“Put *Research Briefs* on Web

“Brief Ray Orbach and BESAC on CSP”

“We (TSG) should do more”

- You gave us compliments on projects’ presentations, new projects’ directions, projects’ selection process, the way we use the “glue” and projects’ graduation process.

CSP's Technology Steering Group (TGS)



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Role of TSG

- Become familiar with the Center's technical activities and comment on their value to DOE Technologies and to industry.
- Provide information from a technology perspective – insight into, and vision of, what is important. Identify technological challenges.
- Influence (steer) the direction of the Center's program. Help develop ideas which can make the Center more effective.
- Take home information and foster closer interactions between the Center, DOE Technologies and industry. Help the Center develop more effective mechanisms for working with DOE Technologies Offices and with industry.
- Become an advocate for, and support the Center's objective to be a model of R and D integration and collaboration within DOE, its Laboratories and with university and industry partners.